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16. Abstract

This is a companion report to Regional Acid Deposition: Models and Physical Processes. This report presents a design and management plan for the development of a Eulerian regional acid deposition model. It first reviews the fundamental physical processes relevant to regional acid deposition and then describes the proposed model system. The principal components (meteorology and chemistry) are discussed in some detail with special emphasis on model initialization and subsystem validation. The total system integration and full validation are presented separately. The management plan section focuses on internal structure, external interactions, and special facility needs. Strongly managed interdisciplinary interactions and intensive "hands-on" working groups for external interactions are suggested.

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The NCAR Acid Deposition Modeling Project

Acid Deposition Modeling Project

NATIONAL CENTER FOR ATMOSPHERIC RESEARCH
BOULDER, COLORADO

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CONTENTS

	Page
List of Figures	v
List of Tables	vii
Preface	ix
EXECUTIVE SUMMARY	1
1. INTRODUCTION TO THE PROBLEM	3
1.1 The Physical Picture	3
1.2 Existing Models and Components of Models	5
1.3 The Chemistry of Acid Generation in the Troposphere	7
1.4 Acid Deposition Model Development and Testing	9
2. OVERVIEW OF THE SYSTEM	10
2.1 The Meteorology System	10
2.1.1 Development of Meteorological Components	14
2.1.2 Model Validation	16
2.2 The Chemistry System	19
2.2.1 The Chemistry-Transport Module	19
2.2.2 Initial and Boundary Conditions	21
2.2.3 Emissions	22
3. SYSTEM INTEGRATION AND VALIDATION	23
4. MANAGEMENT PLAN	26
4.1 Manpower Needs	26
4.2 Internal Management Structure	28
4.3 External Interactions	30
4.4 Facilities for Model System Development	32
5. REFERENCES	32

LIST OF FIGURES

		Page
Figure 2.1	Components of Recommended Acid Deposition Modeling (ADM) System	11
Figure 2.2	Recommended Domain for Preliminary Development and Testing of the ADM System	15
Figure 2.3	The Chemistry-Transport Module	20
Figure 3.1	Recommended ADM System (Physical and Computational Components)	24
Figure 4.1	Proposed Management Structure for ADM System Development	29

LIST OF TABLES

		Page
Table 2.1	Basic Variables Predicted by the Dynamic Model and Derived Variables for Input into the ADM.....	17
Table 2.2	Summary of Meteorological Model Experiments Recommended During Validation Phase of the Project.....	18
Table 3.1	Status of Components of Proposed ADM System.....	27

PREFACE

This report presents a design and management plan for the development of a state-of-the-art Eulerian model for the study of regional acid deposition. This plan directly addresses the findings of our companion report Regional Acid Deposition: Models and Physical Processes (NCAR, 1983).

Our plan integrates recent advances in mesoscale meteorology, tropospheric chemistry, and advanced computing into a scientifically defensible, state-of-the-art regional acid deposition modeling system. The proposed use of an established, proven, mesoscale meteorological model can significantly improve our understanding of the role of transport in acid deposition. The inclusion of fundamental chemical process equations will make it possible to test our understanding of the fundamental transformation processes via comparison with observed data. The focus on statistical and uncertainty analysis will aid the interpretation of modeling results, and hence facilitate the proper assessment of the source-receptor relationship. The modularity of the proposed model system allows the easy and timely incorporation of new results of research sponsored by EPA or other agencies.

This is the second of two reports prepared by the National Center for Atmospheric Research (NCAR) for the Environmental Protection Agency (EPA) under Interagency Agreement No. AD49F2A203 extending from July 1, 1982 to May 31, 1983. It is the collective effort of the members of the NCAR Acid Deposition Modeling Project, but we also acknowledge the broad community of researchers whose work has provided its foundation. We would also like to thank Dr. Kenneth L. Demerjian, EPA Project Officer, whose inspiration and support has made this project possible, and Dr. Wilmot Hess, Director of NCAR, for his enthusiasm and continued interest in the project. Finally, we are also deeply grateful to Daloris Flaming, the administrative assistant for the project, for her continued dedication and perseverance.

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July 1983

The NCAR Acid Deposition Modeling Project

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EXECUTIVE SUMMARY

This document presents a design and management plan for the development of a state-of-the-art Eulerian model for regional acid deposition. This plan is based on the conclusions presented in the companion document entitled Regional Acid Deposition: Models and Physical Processes (NCAR, 1983).

The key conclusions of (NCAR, 1983) are:

- There are fundamental weaknesses in existing models of regional acid deposition, particularly in upper-air transport and dispersion, omissions of detailed chemical reactions, cloud physics, and the treatment of terrain and surface effects.
- Marked improvements are now possible due to recent advances in mesoscale meteorology and tropospheric chemistry; the construction of a comprehensive regional acid deposition model is now feasible.
- The development of such a comprehensive model requires a clearly focused, multidisciplinary group effort under strong scientific leadership.
- The Eulerian framework is most suitable for representing the essential physical and chemical processes in regional acid deposition.

We present here a plan for the integration of recent advances in mesoscale meteorology, tropospheric chemistry, and advanced computing into a scientifically defensible, state-of-the-art regional acid deposition modeling system. A model system developed according to this plan would differ from current models in the following ways:

- It would be based on an established, proven, mesoscale meteorological model and its analysis techniques.
- It would use fundamental chemical process equations to predict the relevant transformations; thus, by comparison with observed data, it would be possible to test our understanding of the fundamental processes.
- It would incorporate the details of both wet and dry deposition.
- Effort would be focused on analyzing the sensitivity of model predictions to uncertainties in chemical initialization and parameterizations.

- Effort would also be focused on the proper statistical interpretation of the model predictions in the context of regional climatology.

- A user-oriented post-processor would facilitate the interpretation and application of the model results.

- It would be modular and highly flexible and would thus allow the easy incorporation of new results of research sponsored by EPA or other agencies.

1. INTRODUCTION TO THE PROBLEM

The Acid Deposition Modeling Project of the National Center for Atmospheric Research has prepared a document entitled Regional Acid Deposition: Models and Physical Processes (NCAR, 1983). It reviews the physical and chemical phenomena that give rise to acidic precipitation and deposition on regional scales from the viewpoint that mathematical modeling of these phenomena is necessary and feasible. While the review is not exhaustive and all-encompassing, it is lengthy. Accordingly, we will introduce the problem by briefly summarizing the contents and conclusions of that report.

The rise of the acid rain (more accurately, acid deposition) problem to public awareness in the United States and Canada has occurred very rapidly and recently. Both public and scientific awareness and activities in Europe, especially Scandinavia, preceded those in North America. Indeed, acid rain is not a new phenomenon; many of the causes and controlling factors and some of the consequences were recognized 100 years ago. Features of the acid rain problem that are new are (a) our perception of the quantitative questions that must be answered to gain a full understanding of the essential chemical and meteorological processes, and (b) our ability to investigate the questions with field- and laboratory-measurement programs and with mathematical models. Similarly, from the point of view of those concerned with the effects of acid rain, there now exist reasonably logical and mature formulations of (c) relationships between ecological systems (and physical structures) and acid deposition that can be investigated quantitatively. Also, as noted above, public awareness of the potential effects and probable causes of acid rain is new, as is the understanding that some kinds of pollution traverse political boundaries.

In the bulk of (NCAR, 1983), we examine the full range of meteorological and chemical processes that are involved in the overall phenomenon; that is, the production and deposition of acidified rain, snow, fog, mist, and dry deposition of acid anhydrides over important inhabited regions such as the east central United States and Canada. We pay particular attention to issues in the study of acid rain through mathematical models. While the scientific questions dictate the kinds of field measurements, laboratory experiments, and model development to be undertaken (all of which are necessary), we are particularly interested in how to develop and employ credible models. By credible models we mean those that are built on basic physical and chemical processes and that can test hypotheses and guide the design and assessment of field measurement programs with the eventual goal of predicting acid deposition rates and source-receptor relationships and of providing reliable estimates of the effects of emission control strategies.

1.1 The Physical Picture

Understanding and modeling the acid rain phenomenon requires one to

recognize a wide range of physical and chemical processes and their interactions. Briefly, these are (a) emissions of materials that cause and regulate acidity in precipitation and deposition, (b) meteorological motions that transport and dilute the emitted substances laterally and vertically, (c) the variety of physical and chemical transformations that alter the physical phase and chemical properties (e.g., valence or oxidation state) of the emitted substances, and (d) the meteorological factors and surface adhesiveness that lead to deposition of the transformed substances. A less well-recognized set of questions surrounds those properties of the Earth's surface that control the rate of uptake of dry materials (e.g., gaseous SO_2 and/or airborne particles).

Because the principal acids in precipitation are sulfuric (H_2SO_4) and nitric (HNO_3), we are most concerned with emissions of sulfur and nitrogen. However, the hydrocarbons and their oxidation products are important reactants in the chemistry which ultimately leads to HNO_3 and H_2SO_4. Estimates of anthropogenic emissions of SO_2 (mostly from coal- and oil-burning electrical power plants and metal-smelting plants) and of NO_x (mostly NO and NO_2 from high temperature combustion processes, including those in auto and truck engines and power plants) are reasonably reliable for the world's industrialized countries. Much less credible, but probably less important, are estimates of natural emissions of organic sulfur gases and of natural NO_x compounds. Natural sources of gaseous NH_3 and particulate NH_4^+, gaseous hydrocarbons, airborne mineral dusts, and lightning-produced NO_x must also be estimated reliably. Minor contributions to precipitation acidity from HCl and organic acids are often negligible.

Whether the key emissions are anthropogenic or natural, they are injected into the atmosphere at or near the Earth's surface, usually within the planetary boundary layer. Accordingly, boundary layer meteorology is at the core of the acid rain problem. The physics of turbulence and convection, diurnal variation in surface heating, terrain geometry, and surface and boundary layer hydrology exert strong control over the initial dispersion of the emitted substances. Further, during the time these substances spend in the boundary layer, their physical environment (e.g., temperature, pressure, humidity, available sunlight) and proximity to surfaces and to other pollutants such as aerosol particles control the rate and type of chemical transformations that occur--and they are markedly different from those that are favored above the boundary layer in the free troposphere. There is perhaps only one important acid precursor or regulator, NO_x from lightning, that does not begin its atmospheric life in the boundary layer, although background tropospheric ozone is central to all tropospheric chemistry.

In dirty or clean air, in the boundary layer and above, chemicals react with each other. The precise rates and types of reactions depend strongly on the local pressure, temperature, available sunlight (both direct and scattered), the presence of liquid and vapor H_2O, and on the local chemical composition (i.e., the spectrum of available chemical coreactants). In Chapter V of (NCAR, 1983), we organize our discussion into categories of homogeneous reactions (gaseous and liquid) and heterogeneous processes and by principal categories of chemical species. Key considerations include the exact rates of transformation (oxidation) of SO_2 and

NO_x into H_2SO_4 and HNO_3, the major pathways of transformation, and the essential controlling agents.

In an oxidizing atmosphere such as that of the Earth, the oxidation of SO_2 and NO_x to H_2SO_4 and HNO_3 is inescapable, given enough time in the atmosphere. Practically, however, it is very important to know what fraction of all of a region's emissions is oxidized and deposited within the region and what fraction of the total is transported long distances (at high altitudes, for example) for eventual deposition onto territories hundreds or thousands of kilometers from the sources. This is to say that a credible description and model of this physical system must include quantitative treatment of material transport and transformation above the boundary layer. Similarly, the factors that limit the rate of surface deposition and uptake of gases (dry deposition) must be treated quantitatively. These include near-ground turbulence, the condition and type of the surface (e.g., vegetation, soils), and the chemical stickiness and reactivity of the relevant substances on the surfaces.

1.2 Existing Models and Components of Models

In Chapter III of (NCAR, 1983), we define, describe, and compare two distinct types of models used for studying long-range transport of air pollutants: Eulerian grid models and Lagrangian trajectory models. Also, because of different goals and problems facing air pollution meteorologists and chemists, it has been useful to develop and employ distinctly different models for air quality modeling (AQM) and acid deposition modeling (ADM). For ADM, we conclude that the three-dimensional nature of the problem and the importance of simulating with adequate generality specific source distributions and eventual control strategies require an Eulerian framework.

Existing ADM's have already contributed to our understanding of the acid rain problem, but a number of phenomena have not been treated fully yet, largely because of the relative youth of the ADM field. Reasonably well-based treatments of each phenomenon have been attempted, but not inside one model; that is, the best available mathematical parameterizations have not been coupled together. Individual models tend to be strong in one respect, but very weak in others. A number of fundamental weaknesses that are widespread, or even ubiquitous, can be mentioned. For example, existing acid deposition models do not allow for mixing of pollutants above the boundary layer. Similarly, no recognition is given to different types of precipitation (rain, snow, dew, etc.) or to the temperature and pH that characterize precipitation scavenging and acid formation. No cloud-chemical processes have been considered so far. Further, fundamental (or elementary) chemical reactions have not been treated with sufficient detail. Instead, linear overall transformation rates have been employed (for example, the rate of conversion of SO_2 to sulfate has been set equal to x% per hour without regard to mechanisms or controlling factors, although seasonal dependence of x is sometimes permitted). No published model has yet included reasonably complete chemical reaction schemes, and nitrogen oxides are usually omitted entirely. Similarly, dry deposition of pollutants has been simulated with fixed deposition velocities, and dependences on winds, surface topography, moisture, and vegetation types have been ignored. Subgrid-scale inhomogeneities in emissions, transport, chemical reaction types

and rates, and deposition have not been included. Consequently, and also because of lack of field data, the verification of ADM's has not progressed very far. Few data and the use of nonmechanistic model parameterizations have led to more model "tuning" in the past than is desirable in the future.

Air quality modeling and regional meteorological modeling are better developed fields than acid deposition modeling. The former have a longer history and a greater data base than the latter. Fortunately, techniques and results from AQM and regional meteorological modeling are valuable for ADM. For example, the experience and results of AQM researchers in dealing with large numbers of chemical reactions can be tapped. Schemes to classify and to reduce systematically the numbers of independent chemical reaction equations offer help to ADM (see especially Chapter V of (NCAR, 1983)). Also, methods of incorporating emissions into AQM's and the AQM emissions data base itself are largely applicable in ADM.

The relative maturity and quantitative nature of regional meteorological modeling as a field can be of enormous benefit to those who seek to develop new, more general and realistic acid deposition models. In Chapter III of (NCAR, 1983), we present an overview of regional meteorological models. A brief history of their goals, methods, and capabilities is outlined and the principal components of these models are identified. Briefly, these are the mathematical or numerical aspects and the more physical features. In the former category, we review the essential features of the spatial grids in these models, the various numerical methods employed to solve the governing partial differential equations, the lateral boundary conditions, and the overriding need for adequate data analysis and data initialization. In each consideration, much of the task at hand in ADM, namely to model accurately the dispersion and transport of pollutants, is closely related to the main purposes of regional meteorological modeling. Thus, the progress and methods in the latter field can be tapped as future ADM's are contemplated and designed.

Similarly, the ways in which the physical aspects of regional meteorological models have been improved and tested will be of benefit to ADM development. These physical aspects include the transports of heat, moisture and momentum at the Earth's surface, in the planetary boundary layer and free troposphere, and the energy sources and sinks that govern the transports. Also included are phase changes of water and the interaction of radiation with clouds and the surface. The fact that these physical phenomena occur on many disparate spatial scales, including scales shorter than a model's grid spacing, necessitates parameterizations--relating the cumulative effect of subgrid-scale phenomena on the fluid flow, for example, to the model-resolvable scales of motion. Parameterizations of surface processes, of planetary boundary layer processes, of condensation and evaporation processes, and of radiative effects of layered clouds in current models are also reviewed, and strong indications of areas ripe for progress are identified. While many of the simpler parameterizations of physical processes now in use in regional meteorological modeling (RMM) are attractive in the early stages of acid deposition model development, it is encouraging to note the progress in RMM toward tractable, improved parameterizations.

Another important consideration in the field of RMM that will be directly useful in ADM is that of objective measures of model skill, i.e., the accuracy of model predictions. In Chapter III of (NCAR, 1983), we review several standard quantitative measures of forecast skill and also summarize the state of the art of RMM's to forecast (precipitation, for example). Clearly, the ability of acid deposition models to forecast deposition patterns (say, annual totals) or deposition amounts in distinct events must be measured objectively. The methods used in RMM will serve as good guides at first.

Because of the great potential for transferring methods and parameterizations from RMM to ADM, we have reviewed components of the former models in some detail, principally in Chapter IV of (NCAR, 1983). First, the need for objective analysis is recognized--irregularly-spaced initial meteorological data must be transformed to provide initial conditions on a model grid. The techniques, quality, computational costs, and history of objective analysis methods are summarized and several case studies are discussed. The related need for data initialization is discussed in similar detail. General physical considerations, mathematical analysis, and experience with meteorological models can indicate general spectral and transient characteristics of data-caused noise. In specific applications (e.g., for a specific regional topography and synoptic situation), there is both sound theory and practical experience to guide the choice of initialization procedure. Accordingly, unneeded computational costs can be avoided. Also, as is true in all methods to solve differential equations, boundary conditions must be specified. Principal techniques now in use in RMM's (spatial damping (or sponge) conditions, wave-radiation conditions) and bounded derivative schemes are reviewed with various applications in mind. Numerical methods and mathematical principles for objective analysis, data initialization, and boundary conditions are also reviewed in Chapter IV of (NCAR, 1983). Once again, the available general theory plus the experience of RMM researchers constitute a well-based foundation for ADM development.

On a more physical side, the essential RMM components mentioned above, surface physics and effects, planetary boundary layer physics and effects, and the thermodynamic and radiative physics and effects of clouds and precipitation are also reviewed. The methods and problems extant in the field of RMM are very close to those that will prevail in ADM.

1.3 The Chemistry of Acid Generation in the Troposphere

As mentioned earlier, the chemical phenomena and reaction sets in existing acid deposition models are far from complete. This is so for many reasons, including the fact that the importance of long-range transport of pollutants has been perceived by the public and its agencies. Accordingly, much work in ADM has focused on the meteorological aspects of transboundary transport. Also, it is true that mechanistic information on the actual chemical processes that transform SO_2 into sulfuric acid and NO_x into nitric acid has appeared very confusing and incomplete until recently. Also, the chemistry of acid generation is more complicated than that of regional chemical oxidants; the former involves gas-phase and aqueous reactions, while the latter is due to gas-phase reactions alone.

Accordingly, our discussions and review of the chemistry of acid generation in Chapter V of (NCAR, 1983) are focused at first on the essential chemistry itself rather than the chemistry now in the existing ADM's. The main categories of the review are gas-phase reactions, aqueous-phase and heterogeneous processes, and photodissociative processes. In any credible ADM, it is extremely important--in fact, essential--to think in terms of reaction mechanisms as opposed to depending completely on parameterizations of overall reaction or transformation rates. For example, it is inadequate to know only the rate at which substance A is transformed to substance C in a mixture as complex and variable as a regionally-polluted atmosphere. Instead of the overall process

$$A \longrightarrow C,$$

we require, instead, knowledge of elementary reaction mechanisms exemplified by

$$A + B \xrightarrow{k} C + D,$$

where the rate k is specific to the two reactants A and B and to reaction conditions (pressure, temperature) and the chemical identities of C and D. Only in this way can a rigorous mechanistic understanding be developed wherein the overall rates of the key transformations and their sensitivities to pollutant and ambient chemical concentrations are predictable. Without it, we would continue to be prey to unknown errors and to criticism of the type that now applies to

$$SO_2 \xrightarrow{\text{rate = x\% per hour}} SO_4^=.$$

For example, this simple and widespread parameterization is inherently linear: the rate of production of $SO_4^=$ is proportional to the gaseous SO_2 concentration. In reality, the supply of the chemicals that actually oxidizes SO_2 to $SO_4^=$ might be limited in certain locations, and little or no $SO_4^=$ production could take place even when large amounts of SO_2 are available there. Similarly, the SO_2-to-$SO_4^=$ conversion rate probably depends on the exact species that is accompanying the oxidation so that the rate, x, is not constant but varies with time. Obviously, analogous fundamental considerations apply to the conversion of NO_x to nitric acid, to the production of photochemical oxidants like ozone and peroxyacetylnitrate, and to the production of SO_2 from biogenic organic sulfides, for example.

The main goals of the very detailed presentations in Chapter V of (NCAR, 1983) are to identify from available research results the principal elementary reaction mechanisms and key species in the gas-phase, aqueous-phase, and heterogeneous reactions that cause and control acid generation. From a complex and encyclopedic list of chemicals and reactions, a smaller, more concise list of chemical variables and processes must be distilled to develop a tractable and useful ADM. From fundamental principles, laboratory data or photochemistry and kinetics, laboratory simulations of complex systems and field data, we can explain the essence of acid generation. These shortened lists of species and processes (elementary reactions when possible) will require further testing, such as zero-dimensional sensiti-

vity calculations. In some cases, such as gas-phase species (i.e., hydrocarbons), the grouping into representative categories has been done in AQM research previously, so only refinements will be needed for ADM development. In other cases, such as solution-phase chemistry, it is not yet completely clear how to achieve conciseness in the reaction list while still simulating the essential features and rates of reactions. This is partly because the role of in-cloud chemistry in generating acids has been appreciated only recently.

Certain clear indications of how to proceed in ADM development do appear in the course of our review. For example, because all gas-phase processes that lead to SO_2 oxidation are initiated by the gas-phase HO radical (in daylight, of course), it is clear that the major processes that control HO concentrations must be embodied in the minimal reaction set for the ADM. Similarly, because of its role in NO_x chemistry and because it is a major source of HO, tropospheric O_3 must be calculated accurately. In the liquid phase, it will be necessary to simulate behavior of O_3, H_2O_2, HO, HO_2, NO_3, and probably O_2^- and N_2O_5. Fortunately, there is a large and talented group of chemists working worldwide on precisely the reactions of interest and there are several international panels who meet regularly to prepare critical reviews of progress in chemical kinetics, so the fundamental data necessary in ADM development are forthcoming or are largely available already.

1.4 Acid Deposition Model Development and Testing

In Chapters IV, V, and VI of (NCAR, 1983), we face many of the issues that arise in the design of a comprehensive model, i.e., one which includes coupled meteorology and chemistry. The key meteorological and chemical processes that are identified in the earlier chapters of the report are stated more concisely in Chapter VI, and certain other phenomena and practical considerations are introduced into the discussion. For example, we discuss the apparent importance of dry deposition of acidic gases and particles, the available methods for its measurement, the controlling physics and chemistry, and how an ADM might treat dry deposition. We also introduce in Chapter VI the questions and facts concerning surface emissions of pollutants and natural sources of acid precursors and of those species that regulate acid generation. Other general features, components, and questions in ADM development are also reviewed and summarized in Chapter VI. These include model resolution, subgrid-scale processes and how to begin to treat them, mathematical and numerical techniques for large comprehensive models, cloud considerations in models with coupled chemistry and physics, and issues in model validation and sensitivity analysis.

While there are many issues and potential problems involved in the development of a comprehensive acid deposition model, it is clear that this field is ripe for progress. The two principal disciplines that are involved, meteorology and atmospheric chemistry, have made dramatic if separate progress recently. Early attempts to include meteorological and chemical processes in integrated models have been useful already, and the experience of the contributing scientists can be tapped. Computational facilities and methods are up to the task. With appropriate amounts of enthusiasm, realism, resources, and teamwork, a new, greatly improved

generation of acid deposition models can be born.

2. OVERVIEW OF THE SYSTEM

2.1 The Meteorology System

To understand the phenomenon of acid deposition, one must understand the atmospheric processes of horizontal and vertical transport, turbulent mixing, and cloud and precipitation formation, in addition to the complex chemistry involved in the formation of acidic material. Because of the transport of gases and aerosols out of the boundary layer by clouds, it is necessary to consider the motions in the entire troposphere in order to determine the transport of chemical species on regional scales. From a scientific point of view, the processes of scale interactions, boundary layer and radiative effects, and cloud and precipitation formation are among the more exciting areas of atmospheric research. From an assessment point of view, the correct modeling of horizontal and vertical transport, turbulent mixing, wet and dry removal, and the possible nonlinear interactions among these processes is essential in evaluating potential control strategies.

The necessary meteorological components of an acid deposition modeling system are shown in Figure 2.1. Input data are routinely available from surface stations, radiosondes, satellites, and aircraft. These different data, at irregularly-spaced points, form the basis for a three-dimensional analysis of the primary meteorological variables (pressure, temperature, water vapor, winds) at regularly-spaced points on a three-dimensional grid. An initialization procedure adjusts these data to a dynamically-consistent set of initial conditions for the dynamic model. This model integrates the equations of motion, the continuity equation for dry air, the theromodynamic equation, and the continuity equation for water forward in time to produce the temporal variation of the meteorological variables in three dimensions. A dynamic model processor then converts these primary data to the meteorological data required by the acid deposition model (ADM). The ADM utilizes these meteorological data to estimate the transport and transformation of the chemical species that contribute to wet and dry acid deposition. Finally, an ADM processor is required to convert the ADM data to estimates of total acid deposition over the temporal and spatial scales of interest.

As reviewed in (NCAR, 1983), considerable progress has been made over the last decade in developing the meteorological components of Figure 2.1. Thus, the time is right for further development and application of these components to the acid deposition problem. Because of the tremendous amount of previous work, we feel it is possible to produce a state-of-the-art meteorological system suitable for applications within a three-year period. In addition, construction of the system with modular components (such as analysis and initialization procedures and physical parameterizations) paves the way for future improvements as scientific advances occur in the components.

While the modular framework for a meteorological model which will provide the necessary meteorological variables as input to the ADM is at the core of our design, another essential component is the validation (or

Figure 2.1
Components of Recommended Acid Deposition Modeling (ADM) System

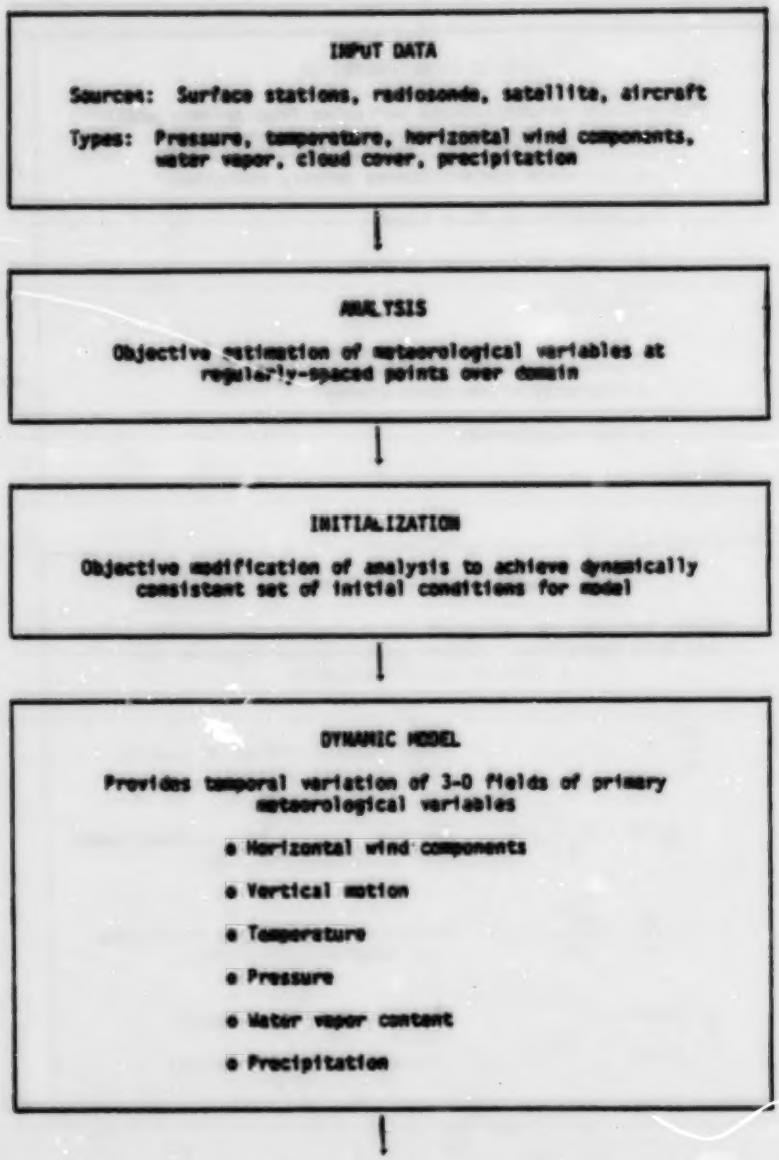

INPUT DATA
Sources: Surface stations, radiosonde, satellite, aircraft
Types: Pressure, temperature, horizontal wind components, water vapor, cloud cover, precipitation
ANALYSIS
Objective estimation of meteorological variables at regularly-spaced points over domain
INITIALIZATION
Objective modification of analysis to achieve dynamically consistent set of initial conditions for model
DYNAMIC MODEL
Provides temporal variation of 3-D fields of primary meteorological variables
• Horizontal wind components
• Vertical motion
• Temperature
• Pressure
• Water vapor content
• Precipitation

Figure 2.1
Components of Recommended Acid Deposition Modeling (ADM) System
(Continued)

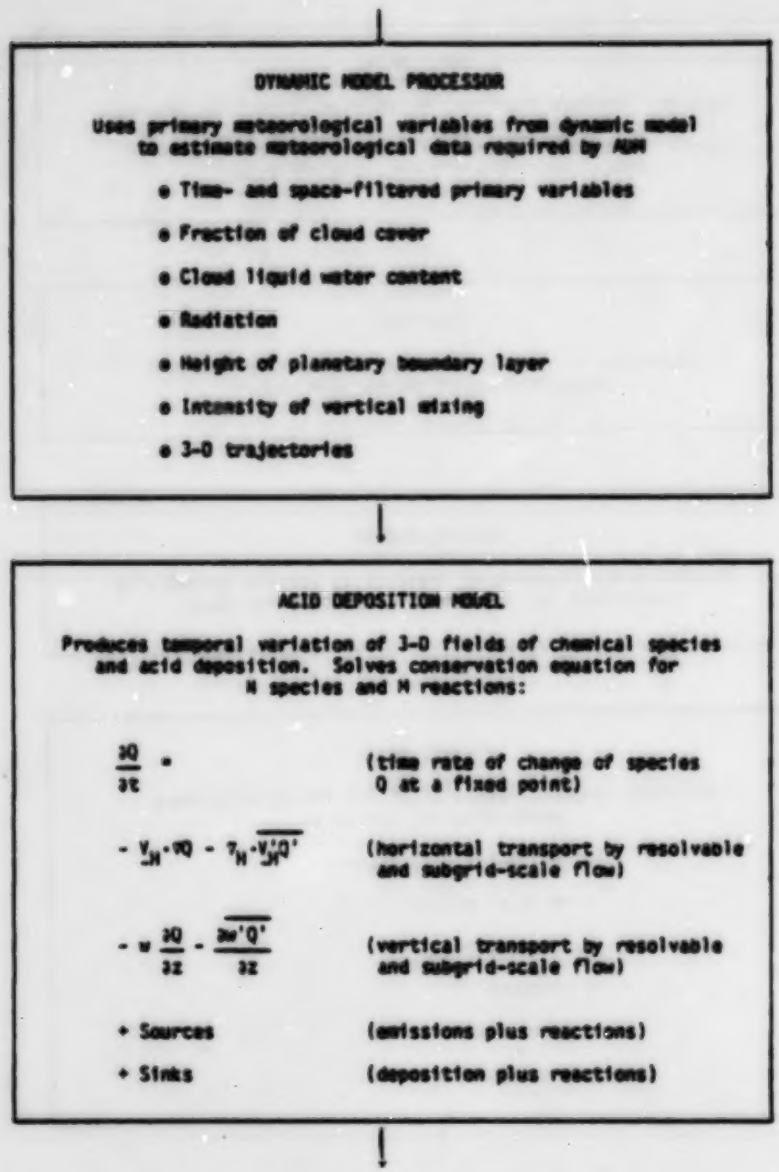
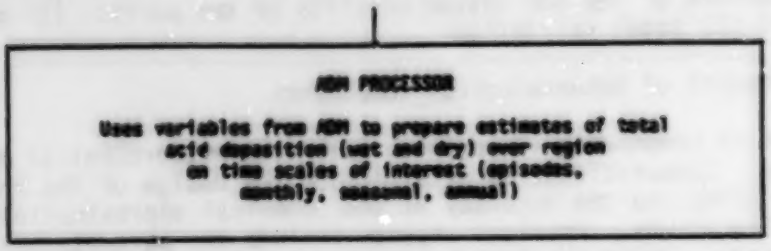

DYNAMIC MODEL PROCESSOR
Uses primary meteorological variables from dynamic model to estimate meteorological data required by ADM
• Time- and space-filtered primary variables
• Fraction of cloud cover
• Cloud liquid water content
• Radiation
• Height of planetary boundary layer
• Intensity of vertical mixing
• 3-D trajectories
ACID DEPOSITION MODEL
Produces temporal variation of 3-D fields of chemical species and acid deposition. Solves conservation equation for N species and N reactions:
$\frac{\partial Q}{\partial t}$ = (time rate of change of species Q at a fixed point)
$-\underline{V}_H \cdot \nabla Q - \nabla_H \cdot \overline{\underline{V}_H' Q'}$ (horizontal transport by resolvable and subgrid-scale flow)
$-w\frac{\partial Q}{\partial z} - \frac{\partial \overline{w'Q'}}{\partial z}$ (vertical transport by resolvable and subgrid-scale flow)
+ Sources (emissions plus reactions)
+ Sinks (deposition plus reactions)

Figure 2.1
Components of Recommended Acid Deposition Modeling (ADM) System
(Continued)


ADM PROCESSOR
Uses variables from ADM to prepare estimates of total acid deposition (wet and dry) over region on time scales of interest (episodes, monthly, seasonal, annual)

testing) of the meteorological model with the goal of determining the inherent uncertainties associated with each component, as well as with the entire system. Application of the complete modeling system in decision-making must recognize the stochastic (uncertain) nature of any simulation or prediction, and determination of the stochastic component introduced by the meteorology is necessary before application of the model to test alternative control strategies. Therefore, the required research on the meteorological component of the ADM system consists of two parts: (1) model development and (2) model validation.

2.1.1 Development of Meteorological Components

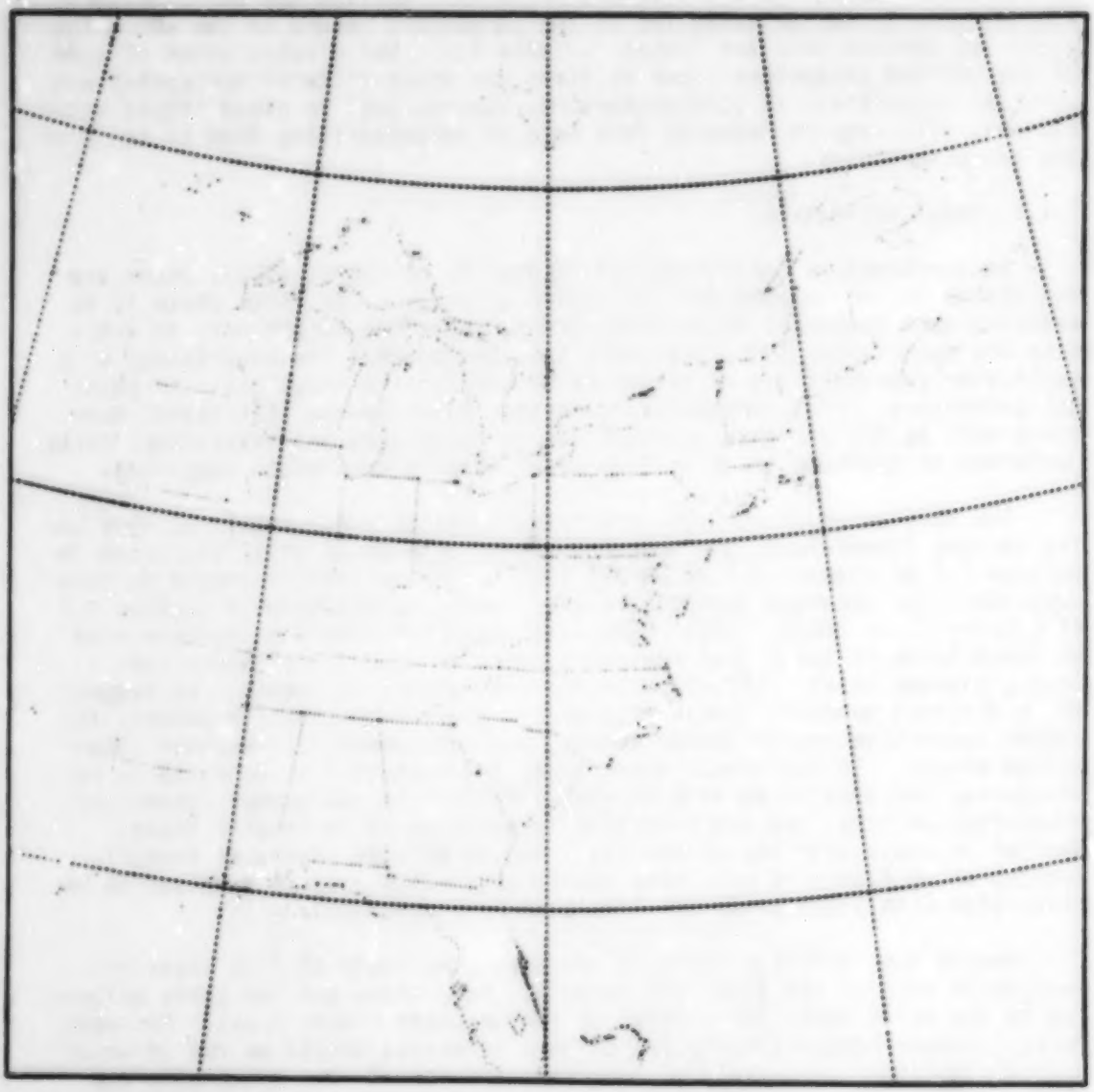
Three major components of regional numerical meteorological models can be identified. Computational aspects include the design of the horizontal and vertical grids and the accuracy of the numerical approximation to the differential equations. Physical aspects include the parameterization of important energy sources or sinks, such as radiation, condensation, and evaporation, and frictional dissipation. Finally, a meteorological model requires initial data and methods of analysis and initialization. These three components are discussed in considerable detail in (NCAR, 1983) in Section 4 of Chapter III and in Chapter IV, so a further review is not required here. Instead, we recommend a specific combination of existing model components for the first-generation ADM system. We emphasize that all of the components proposed here can be added in a modular way, and can therefore be replaced by alternate components. In addition, specific details of the model, such as location of the domain, number of layers, or horizontal resolution, are reasonable estimates only; the system should be designed so that these features can be varied easily for future testing or application. The specifications given here correspond to a medium-resolution model that can be exercised in preliminary tests; it is likely that higher-resolution versions will be required for some applications.

The prototype model recommended for initial development and testing includes 15 layers, a 41 × 41 horizontal grid with a resolution of 80 km, and covers the domain illustrated in Figure 2.2. The relatively coarse grid will allow extensive testing of the model with real data in order to obtain estimates of the model's accuracy and the uncertainties associated with each simulation. Following these preliminary tests, subsequent tests of the model with horizontal resolution of order 20-40 km are recommended if the computer power is available.

The parameterization of planetary boundary layer (PBL) processes should be developed within the framework of a medium-resolution (~ five layers in the lowest kilometer) PBL model in which the vertical fluxes of heat, moisture, and momentum are calculated directly. Not only are such models very general, treating both stable and convective situations and the transition between these states, they are also suitable for providing direct estimates for the ADM of the intensity of vertical mixing, the height of the PBL, and the vertical profiles of wind speed, temperature, and humidity. The PBL formulation must be coupled with a surface energy budget and include a diurnal cycle.

The parameterization of cumulus clouds can be simple at first, and

Figure 2.2
Recommended Domain for Preliminary Development and Testing
of the ADM System



based on empirically-determined vertical profiles of heating and evaporation. The total convective precipitation can be related to the total moisture convergence. An alternative, which could be available in the model as an option, is to neglect the parameterization of convective clouds and instead resolve condensation and evaporation explicitly. The effect of layered nonprecipitating clouds can be considered in the surface energy budget by relating the amount of these clouds to the layer-mean relative humidity.

In addition to developing the analysis and initialization routines and the dynamic model itself, considerable effort will have to be directed toward the development of a processor, which will utilize the basic meteorological data to derive estimates of the parameters needed in the ADM. The basic and derived data are listed in Table 2.1. While calculation of some of the derived parameters (such as time- and space-filtered horizontal and vertical velocities) is straightforward, others, such as cloud liquid water content, will require research into ways of parameterizing them in terms of the basic variables.

2.1.2 Model Validation

As discussed in Section 8.2 of Chapter VI of (NCAR, 1983), there are two phases to the recommended validation strategy. The first phase is to evaluate each component separately, under simplified conditions, to estimate the uncertainty associated with that component. The uncertainty of a particular component can be estimated by varying the input data and physical parameters. From comparative numerical experiments, statistical measures such as the variance and bias can be calculated and statistical tests performed to estimate the significance of varying each model component.

The validation of the complete meteorological model should be done using various conventional and nonconventional methods of skill discussed in Section 4.2 of Chapter III of (NCAR, 1983). The validation should be done separately for separate synoptic weather types, as outlined in Section 8.2 of Chapter VI of (NCAR, 1983). The initial effort should be concentrated on those synoptic types that contribute most to annual acid deposition (e.g., Niemann et al. (1979)). For the preliminary validation, we suggest three distinct synoptic types: (1) winter storm precipitation events, (2) summer convective precipitation events, and (3) summer fair-weather stagnation events. In the winter storm type, precipitation is expected to be widespread and associated with frontal lifting. In the summer convective precipitation type, the precipitation is expected to be locally heavy, smaller in scale than the winter case, and associated with weak frontal systems or no fronts at all. The summer stagnation case is expected to be associated with light winds and little or no precipitation.

During the initial effort, we recommend the study of five cases belonging to each of the first two synoptic types above and two cases belonging to the third type, for a total of twelve cases (Table 2.2A). For each case, a number (approximately 12) of 48-h forecasts should be run in which several important components of the model are varied in a systematic way (Table 2.2B). The statistical aspects of each regional forecast (mean, variance, etc.) can be computed from the 12 forecasts, and the uncertainty associated with each syncptic type estimated from these statistics. In

Table 2.1 Basic Variables Predicted by the Dynamic Model and Derived Variables for Input into the ADM

Basic Variables	Derived Variables
Horizontal wind components	Filtered (in space and time) wind components - for transport
Vertical wind component	Turbulence intensity
Pressure	3-D trajectories
Temperature	Cloud type, amount, and depth
Water vapor	Liquid water content
Precipitation amount	Radiation fluxes
Surface fluxes of heat, moisture, and momentum	Height of planetary boundary layer
	Relative humidity

Table 2.2 Summary of Meteorological Model Experiments Recommended During Validation Phase of the Project

A. Three Synoptic Types:

(1) Winter storm precipitation (5 cases)

(2) Summer convective precipitation (5 cases)

(3) Summer fair-weather, stagnation situation (2 cases)

Total number of cases: 12

B. Variations of Meteorological Model Forecasts:

(1) PBL parameterization

a. Medium resolution, explicit
b. Bulk aerodynamic formulation

(2) Cumulus parameterization

a. Function of total moisture convergence
b. None (explicit calculation of condensation, precipitation)

(3) Surface processes

a. No fluxes of heat or moisture
b. Fluxes computed according to surface energy budget

(4) Radiation (longwave and shortwave)

a. None
b. Interactive with layered clouds

(5) Initialization

a. Analysis, no initialization
b. Analysis, nonlinear normal mode initialization

(6) Comparison of two independently developed models

addition, when the accuracy of forecasts is compared, according to the pairs of forecasts (Table 2.2B), statistically-meaningful statements can be made concerning the impact of varying the individual components. For example, the above set of forecasts will yield 12 forecasts with two different PBL formulations, 12 forecasts with two different initializations, etc. To our knowledge, such organized sensitivity tests with complete diagnostics (measures of skill) have not been conducted. The result will be a well-documented summary of the accuracy and uncertainty associated with the meteorological component of the ADM system.

2.2 The Chemistry System

2.2.1 The Chemistry-Transport Module

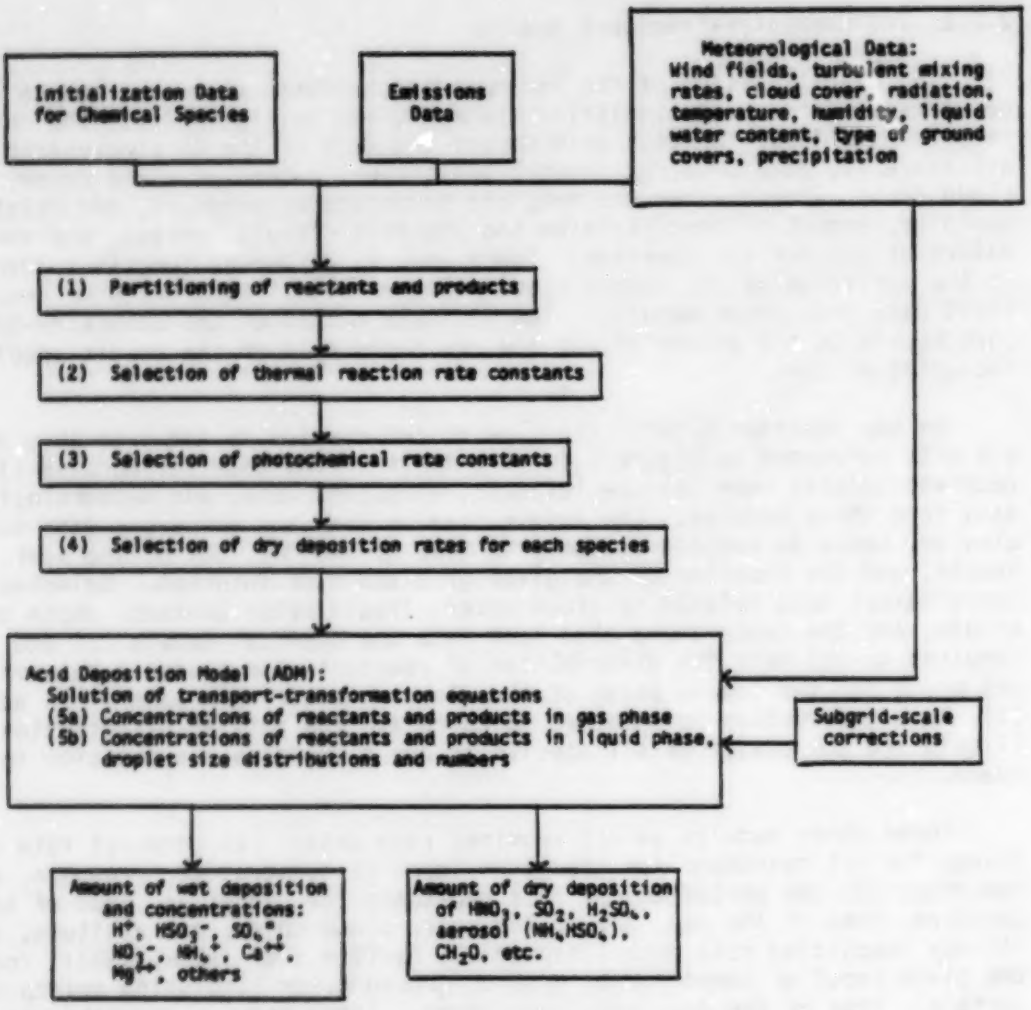
The overall design of the recommended chemistry-transport module can be understood from the simplified diagram given in Figure 2.3. The module receives, as input for each grid square and each of the 15 atmospheric layers above it, data on air transport velocities, extent of cloud cover, the cloud depth, liquid water content, air temperature, pressure, and relative humidity, amount of precipitation and its form (liquid, solid), and the nature of the surface coverage. There are six different functions involved in the operation of the module itself (Figure 2.3). Each of these requires input data from other modules. The ultimate output of the chemistry-transport module is the amount of wet and dry deposition of the acidic species, including H^+ ions.

We may consider briefly the flow of information to and from this module with reference to Figure 2.3. The first of the chemical modules (1) receives initial chemical species data, emissions data, and meteorological data from three modules. The initialization data and emissions data modules are keyed to respond uniquely to time of the day, day of the week, the season, and the location of the given grid scale of interest. Selected meteorological data related to cloud cover, liquid water content, depth of clouds, and the temperature also feed into the chemical module (1) and are required to estimate the distribution of reactants and products between the gas phase and the liquid phase of the cloud water or rain water. In module (1), this information is combined to calculate the initial distribution (liquid and gas phase) of all species at any given time and position in space.

Three other modules select required rate data: (2) chemical rate constants for all reactions for the given input of temperature, pressure, and humidity; (3) the photochemical rate constants for the given input of temperature, time of the day, day of the year, cloud cover, and altitude; and (4) dry deposition rate data (Chapter VI, Section 5 of (NCAR, 1983)) for the given input of temperature, type of ground cover (including moisture on surface), time of the day, and cloud cover. These modules feed the concentration calculation modules (5a) and (5b).

Other meteorological data required for the transport and precipitation calculations at each grid square and atmospheric level, the wind fields (wind velocity components), and the precipitation extent and form (liquid or solid), enter module (5). A subgrid-scale module generates a suitable

Figure 2.3
The Chemistry-Transport Module


Initialization Data for Chemical Species
Emissions Data
Meteorological Data: Wind fields, turbulent mixing rates, cloud cover, radiation, temperature, humidity, liquid water content, type of ground covers, precipitation
(1) Partitioning of reactants and products
(2) Selection of thermal reaction rate constants
(3) Selection of photochemical rate constants
(4) Selection of dry deposition rates for each species
Acid Deposition Model (ADM):
Solution of transport-transformation equations
(5a) Concentrations of reactants and products in gas phase
(5b) Concentrations of reactants and products in liquid phase, droplet size distributions and numbers
Subgrid-scale corrections
Amount of wet deposition and concentrations: H^+, HSO_3^-, $SO_4^=$, NO_3^-, NH_4^+, Ca^{++}, Mg^{++}, others
Amount of dry deposition of HNO_3, SO_2, H_2SO_4, aerosol (NH_4HSO_4), CH_2O, etc.

correction function which also provides input to module (5) to allow for the chemical heterogeneity of certain air masses in which point sources of SO_2 and NO_x are poorly mixed with the bulk of the ambient air containing reactive hydrocarbons, aldehydes, etc. With these combined data, the module (5) solves the coupled differential equations for the transport-transformation and provides concentrations of the reactants and products as a function of time. The concentration of the transient species with very short lifetimes (less than about 1 sec), e.g., HO, HO_2, and RO_2 radicals, is calculated directly from the steady-state relation for the given species at every chosen time interval on the order of minutes.

The output of the chemical transformation-transport module provides the amount of dry deposition of HNO_3, H_2SO_4, aerosol (NH_4HSO_4), SO_2, NO_2, CH_2O, etc. and the amount of wet deposition of H^+, HSO_3^-, $SO_4^=$, NO_3^-, NH_4^+, Ca^{++}, Mg^{++}, and possibly other species of special interest.

The recommended chemical reaction schemes are discussed in detail in Chapter V and in Chapter VI, Section 3, of (NCAR, 1983). The final choice of mechanism will depend upon the results of a preliminary study (first six months) of possible simplified reaction mechanisms based upon the Atkinson et al. (1982) and the Killus and Whitten (1982) gas phase schemes. In the most unfavorable case, gas phase and solution phase reactions required for the chemical module may be about 100 in number, but we expect that some significantly lower number will provide an adequate accuracy. For each of the 15 atmospheric layers above each of the grid squares, our system design requires the storage of the concentration of at least 20 different gas phase species at each of selected time intervals: SO_2, NO, NO_2, O_3, H_2O_2, HNO_3, RH, CH_2O, CH_3CHO, N_2O_5, NO_3, $CH_3COO_2NO_2$ (PAN), NH_3, HO_2NO_2, H_2S, CO, HO, HO_2, CH_3COO_2, RO_2, together with aerosol components: H_2SO_4, NH_4HSO_4, NH_4NO_3, inorganic metal ion-containing species MN(II) and Fe(III), and graphitic carbon; there are also at least 15 different liquid phase species, the concentrations of which must be carried in the memory: S(IV), S(VI), H^+, NO_3^-, NH_4^+, H_2O_2, O_3, CH_2O, $HOCH_2SO_3H$, HO_2NO_2, HO, HO_2, RO_2, Mn(II), Fe(III), and possibly other species, as well as the liquid droplet size distribution.

The output of the chemistry-transport module includes the integral of the amounts of each acidic material (H_2SO_4, HNO_3, H^+, NH_4HSO_4, SO_2, NO_2, HSO_3^-) deposited within each grid square for each of the many simulations designed to duplicate the varied meteorological conditions encountered in the eastern United States.

2.2.2 Initial and Boundary Conditions

Initial distributions and boundary conditions of key gases are likely to have significant impact on the outputs of the acid deposition model. Studies of complete chemical systems involving many species are required to provide estimates of the quantitative impact of variations in the initial concentrations of each species on the final solutions over time periods of a few hours to a few days. It is likely that the distributions of species with lifetimes longer than a day will be affected significantly by their initial values and boundary conditions. Species included in this category are SO_2, $SO_4^=$, NO_x, HNO_3, NO_3^-, O_3, CO, NH_3, H_2O_2, aldehydes, and most

of the volative organic carbons (VOC). Short-lived species such as $O(^1D)$, HO, HO_2, RO, RO_2, NO_3, N_2O_5, PAN, and some other organic radicals are not directly sensitive to initial and boundary conditions because their distributions reach photochemical equilibrium very quickly. However, the short-lived species are affected indirectly by initial and boundary conditions because the concentrations of short-lived species are functions of long-lived species. The results of the quantitative studies mentioned above will help determine what existing data bases are satisfactory for testing the ADM system, as well as provide information concerning necessary measurements in future field programs.

It is clear that the initial conditions for short-lived species can be specified simply at their photochemical equilibrium values once the initial values of long-lived species are determined. For long-lived species, the ideal initial conditions would be the observed values, just as in meteorological models. In reality, this is not possible, because most of the long-lived species are usually not measured in rural areas. Some species such as HNO_3, NO_4^-, NH_3, H_2O_2, aldehydes, and specific hydrocarbons are not even measured routinely in urban centers. Therefore, the initial values of long-lived species must be specified by a combination of extrapolation from limited data and self-consistent model estimates. This is clearly an area where new insights based on analyses with the model would be a necessary bootstrap procedure for the proper initialization. The performance of this procedure can and should be evaluated through additional field measurement programs as will be discussed in Section 3 of this report.

For long-lived species, there is no satisfactory way to specify boundary conditions other than by using measured values, which are not available for most gases. The uncertainty introduced by specification of these species on the lateral boundaries must be a part of the research program. Our strategy would be to set the boundary as far away from the region of interest as the computation cost will allow so that the impact of inaccurately-specified boundary conditions can be minimized.

2.2.3 Emissions

An emissions inventory for a regional acid deposition model provides information needed to investigate major questions on sources of acid deposition. Emissions of the key aerosols and gases involved in acid formation must be considered. Although SO_2 and NO_x are the major acid precursors, several other species significantly influence acid formation. These include VOC and CO, because of their roles as buffering agents in the oxidation process; NH_3, because of its role as a buffering agent in cloud chemistry; and several reduced sulfur species, because of their potential importance as naturally-emitted precursors to acid rain. In addition, primary sulfate emissions could have significant impact on local areas.

It has been concluded (e.g., Galloway and Whelpdale, 1980a,b; Semb, 1978) that anthropogenic emissions of SO_2 exceed natural emissions of gaseous sulfur compounds by at least a factor of ten in eastern North America and Europe. Although this is probably correct, there is large uncertainty in the estimates of natural gaseous sulfur sources. The natural source of NO_x is probably dominated by lightning and soil biogenic activities, al-

though some downward flux of NO_x as well as O_3 from the stratosphere is expected. Quantitative estimates of their source strengths are available, but large uncertainties remain. It is currently believed that anthropogenic NO_x emissions exceed natural emissions by a large factor in eastern North America. Natural sources of VOC, NH_3, and CO are also poorly known. Because of their uncertainties, the natural sources of these species should not be included in the first phase of the ADM system development. Under the National Acid Precipitation Assessment Plan (NAPAP), the National Oceanic and Atmospheric Administration (NOAA) has been assessing the natural sources of gaseous sulfur, NO_x, and NH_3; these results should be incorporated when they are available.

The major man-made emissions data bases are described in Section 1 of Chapter VI of (NCAR, 1983). Reasonably comprehensive data are available for SO_x, NO_x, VOC, and CO. There is no NH_3 emissions inventory for North America, although a state-by-state survey is now being prepared (R. C. Harriss, private communication; R. Husar, private communication). EPA is currently sponsoring Brookhaven National Laboratory (BNL) for compilation of source emissions inventories for acid deposition modeling research.

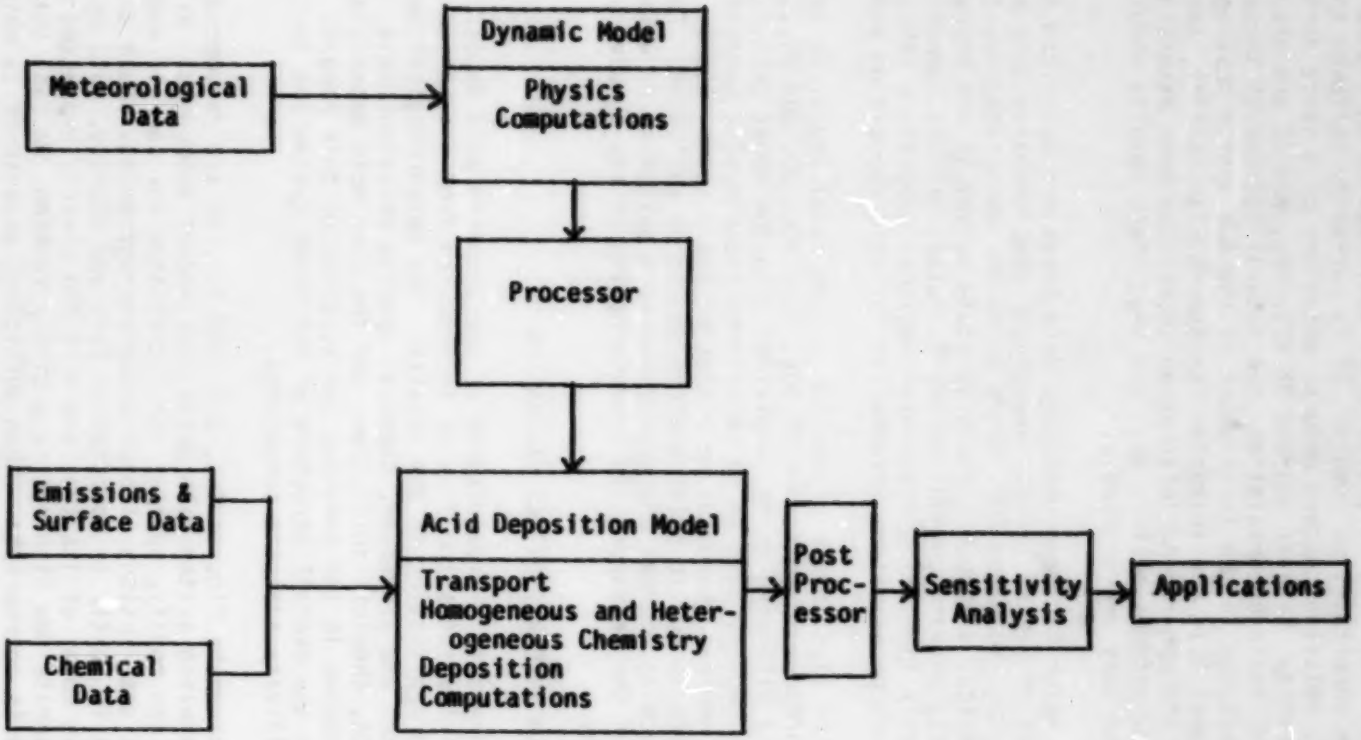
In the first phase of the ADM system development, we suggest including only anthropogenic emissions of SO_x, NO_x, VOC, CO, and NH_3. The emissions data will need to be subdivided into the model grid. Large point sources, however, need to be considered individually because of their impact on chemical phenomena on a smaller scale (Lamb, 1982). Subgrid nonlinear effects due to point sources should be evaluated. Temporal variations (such as diurnal and weekday-weekend patterns) of emissions and their effects on the transport and transformation of key species should also be evaluated.

3. SYSTEM INTEGRATION AND VALIDATION

Figure 3.1, a flow diagram of the proposed acid deposition modeling system, illustrates the flow of information from initiation of the calculation to application of the results. The meteorological data, meteorological model and processor, chemical species emissions data, surface conditions data, chemical initiation, and the core acid deposition model have been discussed in the previous two sections of this report. We shall discuss here the overall structure of the model system and the post-processor and sensitivity analysis components.

As shown by Figures 2.1, 2.3, and 3.1, we are recommending an integrated modeling system with quite independent submodels. Given this system, one can modify, update, and interchange any and all essential physical component descriptions without undue reprogramming. Such an elaborate structure is costly in computation time and storage, but, as the first comprehensive model of its type and with the clearly expressed desire by EPA to incorporate new findings in a timely fashion, we feel this modular structure is appropriate. When sufficient experience is obtained with this system and its components, its developers should look to integration of subsystems to achieve increased computational and storage efficiency. Past experience with other large models at various national laboratories suggests that most large computer codes can be speeded up by factors of 2

Figure 3.1
Recommended ADM System
(Physical and Computational Components)



to 5 depending on the machine and the nature of the code. This effort can be initiated near the end of the third year while validation and model analysis are going on.

The post-processor is essentially a user-oriented interactive graphics package for post-analysis of the ADM system. Past experience tells us that the information flow from three-dimensional models can be simply overwhelming. Computer-assisted analysis is the only logical and feasible solution. Furthermore, one must recognize that not all future users of this ADM system will have or desire to have direct access to the supercomputer where this modeling system must reside. A post-processor designed for smaller computers (minis or even supermicros) can nevertheless yield the end products (e.g., species concentration contours, deposition patterns, scenarios). The user should be able to reorganize the data interactively and carry out simple analyses for scientific and regulatory purposes. This "user-friendly" interface has not been traditional in scientific modeling efforts. Recent advances in micro- and mini-computer systems have demonstrated the great benefits of such an approach to system applications, however. A recent example of such an application is the menu-driven user-interactive chemical kinetics model at NCAR.

Sensitivity analysis is an essential component of the ADM system. As discussed in (NCAR, 1983), there are several techniques in the literature, but none has been applied to acid deposition modeling. Two possible approaches are direct parametric studies and Monte-Carlo-type statistical analysis; they yield different types of information, and both should be used. In direct parametric studies, individual or groups of input variables are modified according to data uncertainties and the model outputs are compared to the reference case. These controlled numerical experiments give very direct cause-effect results, but it is very difficult to use this technique to cover the full range of possibilities. As an alternative, one can use the statistical cases suggested in Section 2.1.2 as the statistical sample and carry out Monte-Carlo-type uncertainty analysis (Stolarski et al., 1978) on the input variables. This gives only a partial answer, however, since such a technique does not point to specific causal relations. Therefore, a judicious application of both techniques is most desirable; this has been shown to be of value in studying problems of stratospheric ozone perturbations, for example.

Validation studies of theoretical models (in particular, computational models) are frequently talked about and proposed but rarely completely carried out. Complex computational models are built precisely because the physical processes to be studied are much too complex for linear analysis. In order to test the accuracy of the model, one must use the ADM system to carry out a detailed analysis of a controlled scenario and then measure the predicted physical quantities. Unfortunately, to our knowledge, this has never been done; field experiments usually are designed in the absence of a comprehensive model. Therefore, questions on the number of variables to be measured, frequency of data collection, geographic coverage, instrument sensitivity, and meteorological conditions are often independently addressed, causing incomplete testing of the model.

We recommend that, beginning in the third year of the project,

planning efforts toward testing the ADM system be initiated using the model system itself as the principal tool for analysis. Although many components of the system would by that time have been tested in the laboratory or in the field, the overall balance and performance of the ADM system still requires testing to add another level of confidence in applications.

Table 3.1 summarizes the status of various components of the proposed ADM system. Many of the meteorological components are well developed but reside in a few operational models. In order to capitalize on the ongoing efforts, this project should seek direct collaboration with one of these efforts. Many components of the proposed acid deposition model are being developed by research groups funded by EPA and others. Close monitoring of these efforts should be established (see following section) to avoid duplication of effort and to facilitate technology transfers. Other components, notably the trace species transport-transformation submodel, the gas-phase and liquid-phase chemistry, and the post-process components, all require dedicated new efforts. As was explained in Section 2.2.1, although several schemes on gas-phase chemistry have been proposed in the literature, they need to be evaluated for suitable implementation in this system. In many ways, this may prove to be more difficult than constructing the original schemes.

4. MANAGEMENT PLAN

4.1 Manpower Needs

The manpower required to build the proposed ADM system will depend on how the effort is partitioned between the prime contractor (i.e., the contractor responsible for the system framework) and the various EPA contractors who will be building specific modules for delivery to the prime contractor. Some of the modules could perhaps most readily be built by the prime contractor, depending on its assembled talents and expertise, while others might more appropriately be completed by EPA contractors already well along on the relevant research.

Nonetheless, we have made some broad estimates of the manpower needed to assemble the proposed ADM system. In so doing, we have assumed the following time table:

June 1, 1983: Project to begin.

Jan. 1, 1985: Progress report on the first generation model.

Jan. 1, 1987: Final report and documentation of the acid deposition model.

During the first year of the project, it will be necessary to incorporate immediately all the "well-developed" (first column, Table 3.1) modules of the proposed ADM system. This includes, most conspicuously, adapting a contemporary, dynamic mesoscale model and its operating packages, such as that described by Anthes and Warner (1978). These well-developed modules would be used in the first-generation system. During the first year, it will also be necessary to begin implementing the modules for which research

Table 3.1
Status of Components of Proposed ADM System

	Well developed; requires implementation	Research in progress	New efforts required
Dynamic Model			
Meteorological data	X		
Objective analysis	X		
Initialization	X		
Numerical methods	X		
Boundary conditions	X		
Surface physics	X		
Planetary boundary layer	X		
Clouds and precipitation			X
Radiation	X		
Processor			X
Validation			X
Synoptic climatology			X
Acid Deposition Model			
Emissions		X	
Surface characteristics		X	
Chemical (species) initialization			X
Transport			X
Cloud submodel		X	
Subgrid processes (point sources, plumes)		X	
Wet deposition		X	
Dry deposition		X	
Gas phase chemistry			X
Liquid phase chemistry			X
Radiation	X		
Heterogeneous processes		X	
Post-Processor			
Post processor			X
Sensitivity analysis		X	
Validation			X
Statistical scenario			X

is in progress (second column). Finally, it will be important to begin work on those modules which require new efforts (third column).

Our estimates of the first-year manpower requirements are (FTE = full-time equivalent):

Incorporate existing modules		2.0 FTE
Complete research in progress		
Dynamical model	2.5 FTE	
Acid deposition model	6.5 FTE	9.0 FTE
Begin new research		
Dynamical model	1.0 FTE	
Acid deposition model	1.0 FTE	
Post-processor	1.0 FTE	3.0 FTE
Estimated total first-year effort		14.0 FTE

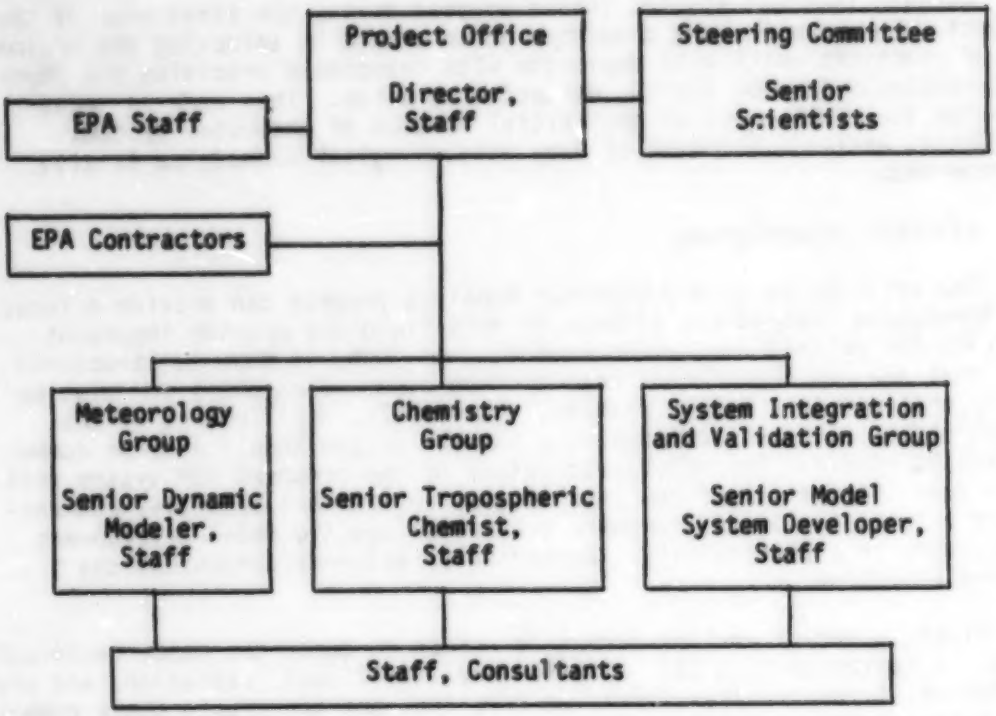
Depending on the existing technical expertise of the prime contractor staff and their preferred scheduling plans, some of the above tasks may have a delayed start. For example, components under development by other research organizations obviously must be included near the completion of those projects. We expect that this initial distribution would be adjusted in later years of the project. However, our past experience with similar projects indicates an even level of manpower requirements over the duration of the project.

4.2 Internal Management Structure

We find the management structure that we adopted during the present project to be appropriate also for building the ADM system, if supplemented with proper interfacing with other EPA contractors and subcontractors. The overall management structure is shown in Figure 4.1. The project director is aided by a Steering Committee which includes senior staff in meteorology, chemistry, and model systems. The director (who should be experienced in building large systems) oversees three groups representing the three key disciplines. Each of these groups is headed by a senior scientist in that specialty. Finally, these three groups draw on the institutional staff, outside consultants, EPA staff, and EPA contractors.

The project director should be the overall scientific leader and manager of the project and the official representative of the project to EPA, EPA contractors, and other cooperating institutions. The project Steering Committee should assist him in the scientific review and planning processes. Particular attention should be devoted to maintaining technical balance and quality. Furthermore, members of the Steering Committee should serve as the senior project liaison with external groups as indicated in

Figure 4.1
Proposed Management Structure for
ADM System Development



Section 4.3. The subgroups should be supervised by their respective senior members with specific details designed to match the stages of program maturity and levels of interactions desired by members of individual groups. It is also recommended that the principal participants be housed together in a centrally-located facility so as to encourage natural interdisciplinary interactions and cooperation.

A detailed work schedule should be prepared within two months of the start of the project. This would allow time to assess the progress and plans of each of the groups preparing submodules for the ADM system.

Certain in-house studies should proceed during the first year of the project. For example, the chemistry group should be selecting the minimal set of reactions which will duplicate with reasonable precision the important reactants for SO_2 and NO_x oxidation to acids. This work is necessary for the development of the initial version of the model system. Similarly, early development of many meteorological submodules is also recommended.

4.3 External Interactions

The anticipated acid deposition modeling program can provide a focus for EPA-funded theoretical efforts in this field and provide important guidance for related field measurements. As such, it must be structured such that new and significant results from other researchers can also be easily included in a timely fashion. Conversely, any findings of the broadly-based research team building the ADM system should also be communicated to others. The modular structure of the proposed ADM system will allow easy integration of new results, but regular and effective communication between the model framework contractor and the model development contractors is a prerequisite. Accordingly, external communications deserve attention.

First, a set of working groups is needed to cover the major technical areas. A tentative list is: dynamic modeling; clouds, radiation, and precipitation; transport-transformation modeling; gas and liquid phase chemistry; heterogeneous processes and deposition; and sensitivity analysis and data bases. The chairman of each working group should be a principal researcher in the subject field. Each group would have about five working scientists in the subject area as members. Each working group would be paired with at least one member of the ADM Steering Committee--i.e, the working groups would be monitored by the overall project director and by the Steering Committee. This structure would assure continuous transfer of information. As the project evolves, some of these working groups may be reorganized, while others may be phased out and new ones added.

Another important role for the disciplinary working groups would be to provide liaison with those external contractors who are developing ADM system modules under EPA contracts. For the overall acid deposition model development to succeed and to meet the desired schedule, a sequence of events must occur according to plan and no hiatuses can be permitted. For example, whoever is responsible for an individual model module must deliver it on schedule, but punctuality alone is not enough. The contractor respon-

sible for model system framework development must communicate with each module development contractor before module delivery to assure compatible goals, formats, and levels of sophistication. Situations in which a module is delivered late or delivered with no prior communication between the parties must be avoided. The goals and contents of each module must be agreed upon or at least commonly understood well before module delivery. To this end, one or more disciplinary working group members, Steering Committee members, and/or the project director should be assigned to be a liaison between the ADM system contractor and the contractor developing each module for the system.

To communicate with an even broader audience and to assimilate emerging scientific knowledge, an annual modeling workshop should be held. Findings of the working groups would be presented at this workshop for general peer review. Because this workshop would be open to interested modelers and other EPA-supported scientists, there would be opportunity for cross-fertilization among modelers, experimentalists, and regulators. As stated in (NCAR, 1983), we believe the Eulerian framework as proposed can best meet the needs of the scientific community in general and EPA in particular, but much has been learned and will continue to be learned from other types of models. Further interaction between modeler and experimentalist is essential for the advancement of our understanding of acid deposition processes. A model-oriented workshop would bring out details of successes and failures of individual efforts, which are often lacking in the usual publications and presentations.

Clearly, close collaboration with the academic community is another essential component of external interactions. Much new information and insight has been brought to the acid deposition modeling field by the more discipline-oriented academic communities. Depending on the nature of the organization which hosts the modeling project, long-term close collaborative efforts with universities clearly can be and should be established.

"Hands-on" cooperation has proven to be an indispensable component of multi-disciplinary research and development projects of this complexity. A flexible management structure should be maintained such that it is possible to invite visitors and send staff to participate actively in collaborative research and development projects. These arrangements can be made on short notice, as soon as the technical needs are apparent, and can last for extended periods. This flexibility will work to the advantage of the project, and allow direct collaboration with others when their modules are being implemented into the model system, for example.

This project must maintain frequent informal contacts and exchanges with EPA staff on all levels. Each year, a mid-year informal oral report on all aspects of the project--technical, financial, and managerial--should be arranged. A formal written report should be prepared and delivered to EPA within one month after the ending of each project year. Technical reports and computer program documentations should be sent on a timely basis. Additional technical support for the EPA project office should also be provided, within the resources of the project.

4.4 Facilities for Model System Development

Essential facilities for developing a model system of the necessary scope are identified as follows. The contractor must have modern digital computer systems with adequate speed and peripheral services, or at least have guaranteed access to such facilities. While computational power (i.e., computer central processor speed and large memory) is essential, input-output devices and facilities for tape handling, etc. are also needed. It is probably also necessary to have midsized computers for processing of input data and for post-processing of model-output fields.

Library facilities and clerical/editorial services must also be considered. Without these, the contractor would be involved in a constant struggle to barely keep pace with scientific developments and with report preparation.

Last, but not least, the host institution should be sufficiently large and prestigious so as to attract and keep top senior scientists as well as bright young staff. For a project of this scope and complexity, a well-balanced mix of experience, dedication, and leadership is the only path to success.

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